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On numerical computation of Coulomb wave functions

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With 2 figures in the text

Introduction

In the theory of proton-proton scattering Coulomb wave functions play a fundamental rôle. For this and similar reasons it seems to be justified to examine methods for their numerical computation. Well-known series expansions have been constructed by SEXL [1] and YOST, WHEELER and BREIT [2]. Further Mathematical Tables Project[1] (now under the direction of Bureau of Standards, Washington, D.C.) is preparing a table of the regular and irregular S-wave functions. With this table it will be possible to obtain any reasonable function value with about 6 digits accuracy.

It is the aim of this paper to give a representation of the Coulomb wave functions with real integrals and to show that they can actually be used for numerical purposes. The formulas might be useful especially in the case when just one or a few function values are needed.

1. The equation which determines the functions in question can be written

$$\frac{d^2 u}{d\varrho^2} + \left(1 - \frac{2\alpha}{\varrho} - \frac{l(l+1)}{\varrho^2}\right) u = 0. \tag{1}$$

A fundamental system is defined with the help of the following boundary conditions:

$$u(0) = 0; \quad u(\varrho)_{\varrho\to\infty} \sim \sin\left(\varrho - \frac{l}{2}\pi + \eta(\varrho, \alpha)\right) \tag{2 a}$$

$$v(\varrho)_{\varrho\to\infty} \sim \cos\left(\varrho - \frac{l}{2}\pi + \eta(\varrho, \alpha)\right). \tag{2 b}$$

$\eta(\varrho, \alpha)$ can be determined from (2 a); then v is defined by (2 b) with the same $\eta(\varrho, \alpha)$.

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[1] I am indebted to Dr. A. N. LOWAN, Math. Tables Project, New York, for placing at my disposal the manuscript of the regular Coulomb wave functions table [3].

Putting

$$u = e^{i\varrho} \cdot \varrho^{l+1} G(\varrho) \tag{3}$$

in (1) we obtain:

$$\varrho (G'' + 2iG') + 2(l+1)(G' + iG) - 2aG = 0. \tag{4}$$

On this equation the usual Laplace-transformation is applied:

$$G = \int \phi(\beta) \cdot e^{\beta\varrho} \cdot d\beta. \tag{5}$$

Observing that $\varrho e^{\beta\varrho} = \frac{d}{d\beta} e^{\beta\varrho}$ we obtain after a partial integration and putting the integrated part and the remaining integrand both equal zero:

$$[(\beta^2 + 2i\beta) \cdot \phi(\beta) \cdot e^{\beta\varrho}]_{s_1}^{s_2} = 0 \tag{6 a}$$

$$\frac{\phi'(\beta)}{\phi(\beta)} = \frac{2l(\beta + i) - 2a}{\beta^2 + 2i\beta} \tag{6 b}$$

where the limits s_1 and s_2 have to be chosen conveniently. Thus

$$\phi(\beta) = (\beta^2 + 2i\beta)^l e^{-2a \operatorname{arctg}(\beta + i)}. \tag{7}$$

The integrated part vanishes when $\beta = 0$, $\beta = -2i$ and $\beta = -\infty$ (since $\varrho > 0$). The first two points are singular, but nevertheless it is possible to choose the integration path from one of the points to the other one. (This could be seen by taking an integration curve, encircling the two points, and then contracting the curve to the double line between $-2i$ and 0.)

Putting $\beta + i = it$ and making some simple reductions we deduce:

$$u = \frac{1}{2^l \cdot l!} \varrho^{l+1} f(a) \cdot \int_0^1 (1 - t^2)^l \cos\left(\varrho t - a \log \frac{1+t}{1-t}\right) dt. \tag{8}$$

$f(a)$ is an amplitude factor which will be determined later. When $a = 0$, u must go over into

$$\sqrt{\frac{\pi\varrho}{2}} \cdot J_{l+\frac{1}{2}}(\varrho).$$

Now we have:

$$\varrho^{l+1} \cdot \int_0^1 (1 - t^2)^l \cdot \cos \varrho t \cdot dt = 2^l \cdot l! \sqrt{\frac{\pi\varrho}{2}} J_{l+\frac{1}{2}}(\varrho)$$

(cf. [4] p. 46), from which we see that $f(0) = 1$.

Analogously if we choose the limits $-\infty$ and 0, we see that we must subtract $i \cdot u$ in order to get the right function v:

$$v = \frac{1}{2^l \cdot l!} \cdot \varrho^{l+1} \cdot g(\alpha) \left\{ \int_0^\infty (1+t^2)^l \, e^{-\varrho t + 2\alpha \operatorname{arctg} t} \, dt - \right.$$

$$\left. - \int_0^1 (1-t^2)^l \sin\left(\varrho t - \alpha \log \frac{1+t}{1-t}\right) dt \right\}. \tag{9}$$

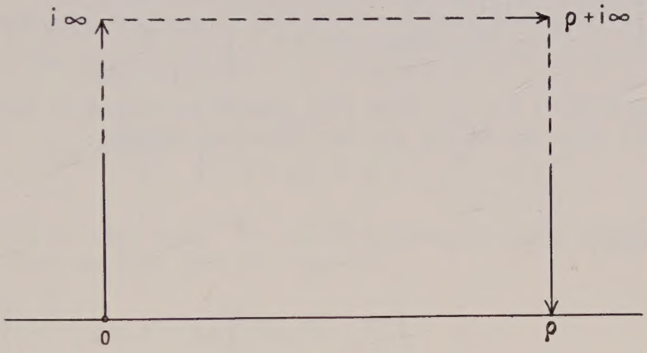

Fig. 1.

2. The asymptotic behaviour for large values of ϱ can be found by writing:

$$u = \frac{1}{2^l \cdot l!} \varrho^{-l} \cdot f(\alpha) \cdot \text{R.P.} \int_0^\varrho (\varrho^2 - x^2)^l e^{ix} \cdot \left(\frac{\varrho + x}{\varrho - x}\right)^{-i\alpha} \cdot dx.^1$$

We replace the integration path along the real axis by

$$(0, i\infty) + (i\infty, \varrho + i\infty) + (\varrho + i\infty, \varrho)$$

(see fig. 1).

Because of the factor e^{ix} the integral between $i\infty$ and $\varrho + i\infty$ drops out and we obtain, putting $x = i\xi$ and $x = \varrho + i\xi$ respectively:

$$u = f(\alpha) \frac{(2\varrho)^{-l}}{l!} \text{R.P.} \left\{ i \cdot \int_0^\infty (\varrho^2 + \xi^2)^l \cdot e^{-\xi + 2\alpha \operatorname{arctg} \frac{\xi}{\varrho}} \cdot d\xi - \right.$$

$$\left. - \int_0^\infty (\xi^2 - 2 i \varrho \xi)^l e^{i\varrho} e^{-\xi} \cdot (2\varrho + i\xi)^{-i\alpha} (-i\xi)^{i\alpha} \cdot i \, d\xi \right\}.$$

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[1] R.P. = real part.

The first integral, being purely imaginary, disappears and we are left with:

$$u = \frac{f(\alpha)}{l!}\,\mathrm{R.P.}\left[\frac{e^{\frac{1}{2}\alpha\pi}}{i}\,e^{i(\varrho-\alpha\log 2\varrho-\frac{1}{2}l\pi)}\int\limits_0^\infty\left(1+\frac{i\,\xi}{2\,\varrho}\right)^{l-i\alpha}\xi^{l+i\alpha}\,e^{-\xi}\,d\,\xi\right].$$

For large values of ϱ the factor $1+\dfrac{i\,\xi}{2\,\varrho}$ may be replaced by unity, and the integral reduces to $\Gamma(i\,\alpha+l+1)$. Thus:

$$u \sim \frac{f(\alpha)\,e^{\frac{1}{2}\alpha\pi}}{l!}\sqrt{\frac{(1+\alpha^2)(4+\alpha^2)\cdots(l^2+\alpha^2)\,\pi\,\alpha}{\mathrm{sh}\,\pi\,\alpha}}\cdot\sin\left(\varrho-\alpha\log 2\,\varrho-\tfrac{1}{2}\,l\,\pi+\eta_l\right)$$

where $\eta_l = \arg\Gamma(i\,\alpha+l+1)$. Now $f(\alpha)$ should be chosen to make the amplitude unity, and then we finally get the following formula:

$$u_l = 2^{-l}\sqrt{\frac{1-e^{-2\pi\alpha}}{2\pi\,\alpha\,(1+\alpha^2)\cdots(l^2+\alpha^2)}}\,\varrho^{l+1}\,\cdot$$

$$\cdot\int\limits_0^1(1-t^2)^l\cos\left(\varrho\,t-\alpha\,\log\frac{1+t}{1-t}\right)d\,t. \qquad (10)$$

In an analogous way we get, finding $g(\alpha) = f(\alpha)$:

$$v_l = 2^{-l}\sqrt{\frac{1-e^{-2\pi\alpha}}{2\pi\,\alpha\,(1+\alpha^2)\cdots(l^2+\alpha^2)}}\,\varrho^{l+1}\left[\int\limits_0^\infty(1+t^2)^l\,e^{-\varrho t+2\alpha\,\mathrm{arctg}\,t}\cdot d\,t\,-\right.$$

$$\left.-\int\limits_0^1(1-t^2)^l\cdot\sin\left(\varrho\,t-\alpha\,\log\frac{1+t}{1-t}\right)d\,t\right]. \qquad (11)$$

The formulas (10) and (11) are, of course, essentially identical with the well-known integral representations, given e.g. in MOTT–MASSEY [5]. It does not seem to have been pointed out before, however, that numerical computation actually can be performed on the basis of the formulas above. We will return to this later and also give some examples.

3. For reference we also give the behaviour at the origin. Then we need the integral

$$I = \int\limits_0^1(1-t^2)^l\cdot\cos\left(\alpha\,\log\frac{1+t}{1-t}\right)d\,t = \tfrac{1}{2}\int\limits_{-1}^{+1}(1-t^2)^l\cdot\left(\frac{1+t}{1-t}\right)^{i\alpha}d\,t.$$

After the substitution $t = 2x - 1$ the integral transforms to:

$$I = 2^{2l} \int_0^1 x^{l+ia} (1 - x)^{l-ia}\, dx = 2^{2l} \cdot \frac{\Gamma(l + 1 + ia) \cdot \Gamma(l + 1 - ia)}{\Gamma(2l + 2)} =$$

$$= \frac{2^{2l}}{(2l + 1)!} \cdot \frac{(1 + a^2) \cdots (l^2 + a^2)\, \pi a}{\operatorname{sh} \pi a}.$$

The remaining integrals needed are elementary.

Thus we have the following approximate formulas for small values of ϱ:

$$u_l \sim \frac{2^l}{(2l + 1)!} \cdot \sqrt{\frac{2\pi a (1 + a^2) \cdots (l^2 + a^2)}{e^{2\pi a} - 1}} \cdot \varrho^{l+1} \tag{12 a}$$

$$v_l \sim \frac{(2l)!}{2^l} \cdot \sqrt{\frac{e^{2\pi a} - 1}{2\pi a (1 + a^2) \cdots (l^2 + a^2)}} \cdot \varrho^{-l}. \tag{12 b}$$

(12 a) and (12 b) can easily be obtained from the series expansions (cf. e.g. [5], p. 53). Now we also find the equalities:

$$\left.\begin{array}{l} \lim\limits_{\varrho \to 0} \dfrac{d u_l}{d \varrho} v_l = \dfrac{l + 1}{2l + 1} \\[2ex] \lim\limits_{\varrho \to 0} u_l \dfrac{d v_l}{d \varrho} = - \dfrac{l}{2l + 1} \\[2ex] \lim\limits_{\varrho \to 0} \dfrac{u_l v_l}{\varrho} = \dfrac{1}{2l + 1} \end{array}\right\} \tag{13}$$

4. In the applications the case $l = 0$ will be of special interest. The function v_0, however, contains an integral over an infinite interval, so we make the following transformation: $\xi = e^{-\varrho t}$ and replace ξ by t. Then we get:

$$u_0 = \sqrt{\frac{1 - e^{-2\pi a}}{2\pi a}} \cdot \varrho \int_0^1 \cos\left(\varrho t - a \log \frac{1 + t}{1 - t}\right) dt \tag{14 a}$$

$$v_0 = \sqrt{\frac{1 - e^{-2\pi a}}{2\pi a}} \cdot \int_0^1 \left[e^{2a \operatorname{arctg} \frac{\log 1/t}{\varrho}} - \varrho \sin\left(\varrho t - a \log \frac{1 + t}{1 - t}\right)\right] \cdot dt. \tag{14 b}$$

Both integrands are finite, and even the singularity in $t = 1$ will cause no trouble at the numerical computation. The integrand of (14 a) is presented in fig. 2.

A few function values have been computed for $a = \frac{1}{2}$ and some of them could be compared with the corresponding values from the table [3]. The

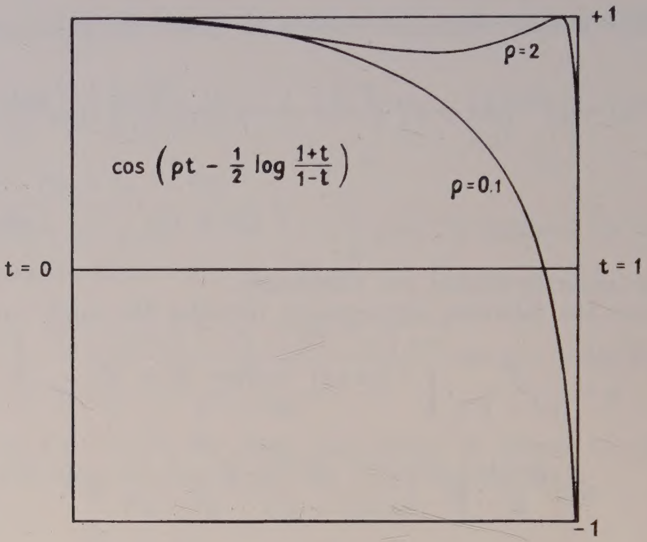

Fig. 2.

numerical integration was performed by Simpson's rule and rather large intervals. There would be but little difficulty to increase the accuracy considerably. The table below gives the result.

$\alpha = \frac{1}{2}$.

ϱ	u_0 (comp.)	u_0 (tab.)	Diff. %	u_1 (comp.)
0.1	0.039511	0.039519	0.020	0.00143785
0.6	0.284800	0.284742	0.020	0.056582
1.0	0.516583	0.516601	0.003	0.162767
2.0	1.021184	1.021120	0.006	0.618514

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